LATTICE FIELD THEORY 2

More Numerical Methods in QM

Scalar Field Theory

Lattice Gauge Theory

Andreas S. Kronfeld

1 September 2003

More on Path Integrals

Last time we derived an expression for the (imaginary time, $T \to -iT$) propagator

$$\langle x_T | e^{-\hat{H}T} | x_0 \rangle = \lim_{N \to \infty} \int \mathcal{D}x_N \, e^{-S(\{x_i\}_N)}, \qquad \mathcal{D}x_N = \prod_{i=1}^{N-1} dx_i \sqrt{\frac{m}{2\pi a}},$$

$$S = a \sum_{i=0}^{N-1} \left[\tfrac{1}{2} m \left(\frac{x_{i+1} - x_i}{a} \right)^2 + V(x_i) \right].$$

The left-hand side obeys a composition law when tacking two paths together:

$$\langle x_{T'+T} | e^{-\hat{H}(T'+T)} | x_0 \rangle = \int dx_T \, \langle x_{T'+T} | e^{-\hat{H}T'} | x_T \rangle \langle x_T | e^{-\hat{H}T} | x_0 \rangle$$

So does the right-hand side:

$$\int \mathcal{D}x_{N'+N} \, e^{-S(\{x_i\}_{N'+N})} = \int dx_N \int \mathcal{D}x_{N'} \, e^{-S(\{x_i\}_{N'})} \int \mathcal{D}x_N \, e^{-S(\{x_i\}_N)},$$

even without taking the limit of infinite N, N'.

Furthermore, an operator $\hat{Q} = Q(\hat{x}) = \int dx |x\rangle Q(x) \langle x|$, acting at time t, $0 < t < T$,

$$\langle x_T | e^{-\hat{H}(T-t)} Q(\hat{x}) e^{-\hat{H}t} | x_0 \rangle = \int \mathcal{D}x \, Q(x_t) \, e^{-S(\{x_i\})}$$

and similarly for several operators inserted at various different times.

In field theories, we do not have 1 degree of freedom. We have many.

It is impractical to study the dependence of the wave function on all of them.

So let us set $x_T = x_0$ and integrates over x_0, yielding the "partition function"

$$Z = \int \mathcal{D}x \, e^{-S}, \qquad \mathcal{D}x = \prod_{i=0}^{N-1} dx_i,$$

now with N integrations.

The parallel with statistical mechanics can be pursued further by introducing

$$\langle Q(x_t) \rangle = \frac{1}{Z} \int \mathcal{D}x \, Q(x_t) \, e^{-S(\{x_i\})}$$

$$\langle Q_1(x_{t_1}) Q_2(x_{t_2}) \rangle = \frac{1}{Z} \int \mathcal{D}x \, Q_1(x_{t_1}) Q_2(x_{t_2}) \, e^{-S(\{x_i\})}$$

$$\langle Q_1(x_{t_1}) Q_2(x_{t_2}) \rangle_c = \langle Q_1(x_{t_1}) Q_2(x_{t_2}) \rangle - \langle Q_1(x_{t_1}) \rangle \langle Q_2(x_{t_2}) \rangle$$

The clash of the notation $\langle \bullet \rangle$ with Dirac notation is unfortunate, but conventional.

For large T \hspace{6cm} Proofs as exercises.

$$Z \xrightarrow{\text{large } T} e^{-E_0 T}$$

$$\langle Q(x_t) \rangle \xrightarrow{\text{large } T} \langle 0 | Q(\hat{x}) | 0 \rangle$$

gives you the vacuum energy E_0 and vacuum expectation value (vev).

Not miraculous. Recall scattering theory, with propagators out to $T(1 - i0^+)$.

For large T (and $x_{t_1} - x_{t_2} = ja$)   Proof as exercise.

$$\langle Q_1(x_{t_1})Q_2(x_{t_2})\rangle_c \xrightarrow{\text{large } T} \sum_{n\neq 0} \langle 0|Q_1(\hat{x})|n\rangle\langle n|Q_2(\hat{x})|0\rangle e^{-(E_n-E_0)ja}$$

$$+ \sum_{n\neq 0} \langle 0|Q_2(\hat{x})|n\rangle\langle n|Q_1(\hat{x})|0\rangle e^{-(E_n-E_0)(T-ja)},$$

gives you the excited-state energies E_0 and vacuum $\to$ 1-particle matrix elements.

For large ja and/or $T - ja$ Proof as exercise.

$$\langle Q_1(x_{t_1})Q_2(x_{t_2})\rangle_c \xrightarrow{\text{large } T} \langle 0|Q_1(\hat{x})|1\rangle\langle 1|Q_2(\hat{x})|0\rangle e^{-(E_1-E_0)ja}$$
$$+ \langle 0|Q_2(\hat{x})|1\rangle\langle 1|Q_1(\hat{x})|0\rangle e^{-(E_1-E_0)(T-ja)},$$

thus isolating properties of the first excited-state $|1\rangle$.

If (by symmetry or clever design) $Q_i(\hat{x})|1\rangle = 0$, then higher excited states $|2\rangle \cdots$.

In field theory, these energies are nothing but masses of particles.

Monte Carlo Integration

Choose a random configuration of the x_i, which we can denote $\{x_i\}^{(c)}$, and we can generate C such configurations. Then

$$Z = \int \mathcal{D}x\, e^{-S} = \lim_{C \to \infty} \left(\frac{m}{2\pi a}\right)^{N/2} \sum_{c=0}^{C-1} \exp\left[-S\left(\{x_i\}^{(c)}\right)\right],$$

$$\int \mathcal{D}x\, f(\{x_i\})e^{-S} = \lim_{C \to \infty} \left(\frac{m}{2\pi a}\right)^{N/2} \sum_{c=0}^{C-1} f(\{x_i\}^{(c)}) \exp\left[-S\left(\{x_i\}^{(c)}\right)\right].$$

An estimate of the left-hand side is achieved for C finite.

From now on we use finite C, and omit the normalization factor $(m/2\pi a)^{N/2}$, which drops out of correlation functions.

This method is hopeless for large N. S is extensive, many configurations have $S \sim N$; they are a waste of time.

The remedy is called importance sampling.

Don't choose all configurations with equal weight, choose them with weight e^{-S}.

This is possible because S is real and bounded below.　　　Hence imaginary time!

Then

$$\frac{1}{Z} \int \mathcal{D}x\, f(\{x_i\}) e^{-S} \approx \frac{1}{C} \sum_{c=0}^{C-1} f(\{x_i\}^{(c)}).$$

converging to be exact as $C \to \infty$.

Quantum theory has been reduced to the design of random number generators, for many variables, with distribution e^{-S}.

A Simple Method

Perhaps the simplest method to generate the desired distribution is the Metropolis method.

Requires only $e^{-S} \geq 0$.
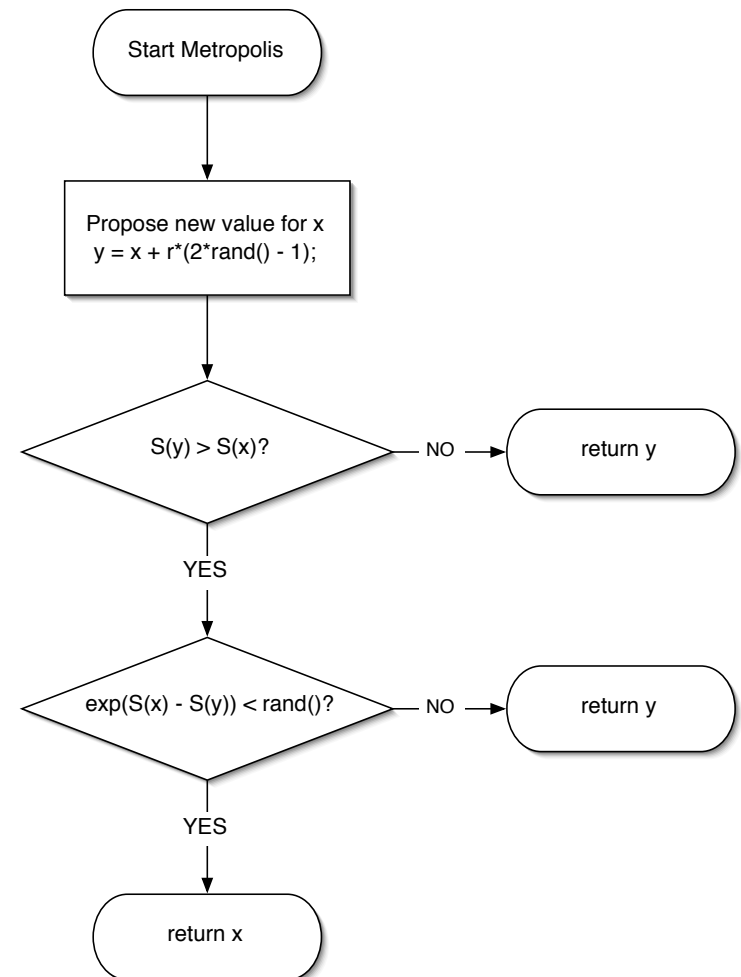
Visit each x_i in turn, and follow the flow chart.

$\texttt{rand}() \in [0, 1)$

Choose r to accept ~ 40–50% of updates.

For more complicate (sets of) degrees of freedom only the proposed update must change.

May also update x_i several times, before proceeding to $i + 1$.

```
Start Metropolis

Propose new value for x
y = x + r*(2*rand() - 1);

S(y) > S(x)?   --NO-->   return y
   |
  YES
   |
exp(S(x) - S(y)) < rand()?   --NO-->   return y
   |
  YES
   |
return x
```

Necessary *vs.* Sufficient for Monte Carlo

The aim of any algorithm is to generate a transition rule $T(\{x\} \to \{y\})$ so that the probability density is (eventually) $P(\{x\}) \propto e^{-S(\{x\})}$.

Start with an initial distribution $P(\{x\}, 0)$. The transition rule $T(\{x\} \to \{y\})$ changes the distribution from $P(\{x\}, c)$ to $T(\{x\} \to \{y\})$ independent of c.

$$P(\{x\}, c+1) = P(\{x\}, c) - \int \mathcal{D}y\, P(\{x\}, c) T(\{x\} \to \{y\})$$

$$+ \int \mathcal{D}y\, P(\{y\}, c) T(\{y\} \to \{x\})$$

The steady state (if it exists) has $P(\{x\}, c)$ independent of c.

$$\int \mathcal{D}y\, P(\{x\}) T(\{x\} \to \{y\}) = \int \mathcal{D}y\, P(\{y\}) T(\{y\} \to \{x\}) \qquad \text{necessary}$$

$$P(\{x\}) T(\{x\} \to \{y\}) = P(\{y\}) T(\{y\} \to \{x\}) \qquad \text{sufficient}$$

The last (unintegrated) condition is called detailed balance. It is easier to satisfy.

Metropolis and Detailed Balance

We now check the Metropolis satisfies detailed balance, re-written

$$\frac{T(\{x\} \to \{y\})}{T(\{y\} \to \{x\})} \stackrel{!}{=} \frac{P(\{y\})}{P(\{x\})} = e^{-[S(\{y\}) - S(\{x\})]} = e^{-\Delta S}$$

Three cases:

$S(\{y\}) = S(\{x\})$	$S(\{y\}) > S(\{x\})$	$S(\{y\}) < S(\{x\})$
always accept	$0 < e^{-\Delta S} < 1$	$T(\{x\} \to \{y\}) = 1$
both Ts $= 1$	"accept if $R \leq e^{-\Delta S}$"	$T(\{y\} \to \{x\}) = e^{\Delta S}$
$e^{-\Delta S} = 1$	accepts fraction $e^{-\Delta S}$	
	$T(\{x\} \to \{y\}) = e^{-\Delta S}$	
	$T(\{y\} \to \{x\}) = 1$	

In all three cases, Metropolis satisfies detailed balance.

Statistical Uncertainties

With Monte Carlo integration, there are statistical errors that fall as C^{-1}.

Let the average in the finite ensemble be written

$$\overline{f(\{x_i\})} := \frac{1}{C} \sum_{c=0}^{C-1} f(\{x_i\}^{(c)}).$$

so $\overline{f(\{x_i\})}$ estimates $\langle f(\{x_i\}) \rangle$.

The central limit theorem says that $\overline{f(\{x_i\})}$ fluctuates around $\langle f(\{x_i\}) \rangle$ with variance

$$\sigma^2(f) = \frac{1}{C-1} \left[\overline{f^2} - \overline{f}^2 \right].$$

(Think of repeating a Monte Carlo of C configurations many times, and drawing the histogram of $\overline{f}$.)

Indeed, statistical fluctuations are correlated

$$\sigma^2\left(f_i, f_j\right) = \frac{1}{C-1}\left[\overline{f_i f_j} - \overline{f_i}\,\overline{f_j}\right].$$

For example, $f_t = Q(x_t)Q(x_0)$ and f_{t+u}.

In field theory, we can gain some intuition about the fluctations, because

$$\overline{f_i f_j} - \overline{f_i}\,\overline{f_j} \approx \langle f_i f_j\rangle - \langle f_i\rangle\langle f_j\rangle.$$

In practice, similar quantities (like successive times of a correlation function) fluctuate together.

Statistical errors often cancel somewhat when forming ratios and differences.

Statistical Errors for Masses, etc.

Usually we are interested in energies or quantum-mechanical matrix elements.

For example, the energy difference can be extracted from

$$m_{\text{eff}}(t) = -\ln \frac{\langle Q_1(x_{t+1})Q_2(x_0)\rangle_c}{\langle Q_1(x_t)Q_2(x_0)\rangle_c}$$

Independent of $t \Leftrightarrow$ one state dominates.

Logarithm does not commute with $\langle \bullet \rangle$.

To estimate the statistical error on m_{eff}, we really need many ensembles.

In the bootstrap method, new pseudo-ensembles are generated from the original, by drawing configurations at random, allowing repeats.

Bootstrap can be wrapped around an arbitrarily complicated analysis.

Scalar Field Theory on a Lattice

In quantum mechanics the action in the path integral is

$$S = a \sum_{i=0}^{N-1} \left[\tfrac{1}{2}m \left(\frac{x_{i+1} - x_i}{a} \right)^2 + V(x_i) \right].$$

where the velocity dx/dt is replace by a discrete approximation.

The simplest scalar field theory simply repeats this replacement for all d directions,

$$S = a^d \sum_n \left[\sum_{\mu=1}^{d} \tfrac{1}{2} a^{-2} \left(\phi_{n+e^{(\mu)}} - \phi_n \right)^2 + V(\phi_n) \right].$$
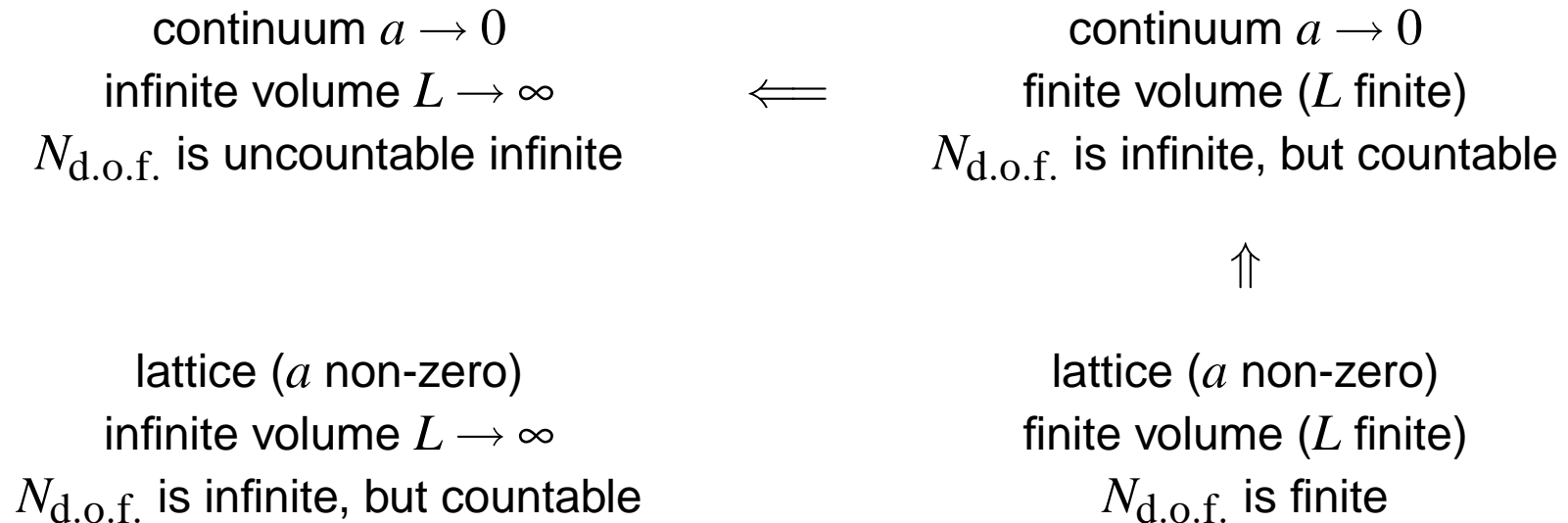
where $e^{(\mu)}$ is a unit vector in the μ direction, and $n \in \mathbb{Z}^d$.

This is a square, cubic, or hypercubic lattice for $d = 2, 3, 4$.
Dimensionful spacetime labels $x = na$.

What does the lattice do to the field theory?

In the spatial directions, $L = Na$ be the physical size of the box. Then

<div style="display:flex">

continuum $a \to 0$
infinite volume $L \to \infty$
$N_{\text{d.o.f.}}$ is uncountable infinite

$\Longleftarrow$

continuum $a \to 0$
finite volume (L finite)
$N_{\text{d.o.f.}}$ is infinite, but countable

$\Uparrow$

lattice (a non-zero)
infinite volume $L \to \infty$
$N_{\text{d.o.f.}}$ is infinite, but countable

lattice (a non-zero)
finite volume (L finite)
$N_{\text{d.o.f.}}$ is finite

</div>

No divergences if $N_{\text{d.o.f.}}$ is finite, *i.e.*, if a non-zero and L finite.

Ultraviolet and infrared divergences do not appear in combinations of *physical* quantities. Instead $g_0^2 = g_0^2(a)$.

Free Lattice Field Theory

The kinetic terms may be re-written

$$\sum_n \left(\phi_{n+e^{(\mu)}} - \phi_n \right)^2 = \sum_n 2\phi_n^2 - 2\phi_n \phi_{n+e^{(\mu)}} = \sum_n 2\phi_n^2 - \phi_n \left(\phi_{n+e^{(\mu)}} + \phi_{n-e^{(\mu)}} \right)$$

analogous to integrating by parts $(\partial_\mu \phi)^2 \to -\phi \partial_\mu^2 \phi$.

So we will take the lattice Lagrangian (or Lagrange density) to be

$$\mathcal{L}_n = a^{-2} \frac{1}{2} \sum_\mu \phi_n (t_\mu + t_{-\mu} - 2) \phi_n - V(\phi_n), \quad S = -a^d \sum_n \mathcal{L}_n, \quad t_{\pm\mu} \phi_n = \phi_{n \pm e^{(\mu)}}.$$

For free fields $V(\phi) = \frac{1}{2} m_0^2 \phi^2$. In momentum space, the propagator is

$$G(p)^{-1} = \hat{p}^2 + m_0^2$$

where $\hat{p}^2 a^2 = \sum_\mu \frac{1}{2} (e^{ip_\mu a} + e^{-ip_\mu a} - 2) = \sum_\mu [2\sin(\frac{1}{2} p_\mu a)]^2 = \sum_\mu \hat{p}_\mu^2 a^2$.

Fourier transform from p_4 back to t:

$$G(t,\vec{p}) = \int \frac{dp_4}{2\pi} \frac{e^{ip_4t}}{\hat{p}_4^2 + \hat{\vec{p}}^2 + m_0^2} = \int \frac{dp_4}{2\pi} \frac{a^2 e^{ip_4t}}{2 + a^2(\hat{\vec{p}}^2 + m_0^2) - 2\cos p_4 a}$$

$$= \oint \frac{dz}{2\pi i} \frac{az^{|t|/a}}{2z\cosh Ea - 2(z^2+1)}, \qquad z = e^{\mathrm{sign}(t)ip_4a}$$

$$= \frac{ae^{-E|t|}}{2\sinh Ea} \qquad\qquad \text{expected} \quad \frac{e^{-|t|(\vec{p}^2+m^2)^{1/2}}}{2E}$$

where $\cosh Ea = 1 + \frac{1}{2}a^2(\hat{\vec{p}}^2 + m_0^2)$.

Here we have defined the energy through the fall-off of the correlation function.

$$\langle \phi(t,\vec{p})\phi(0,\vec{q}) \rangle = (2\pi)^{d-1}\delta(\vec{p}-\vec{q})G(t,\vec{p})$$

We see that discretization effects distort the energy.
They also change the normalization so it is not quite canonical.

Lattice Gauge Theory

Now suppose we have a complex (*i.e.*, charged scalar field).

Suppose it transforms under some gauge group as

$$\phi(y) \to g(y)\phi(y), \qquad \phi^\dagger(x) \to \phi^\dagger(x)g^\dagger(x), \qquad g^\dagger = g^{-1}.$$

In the Lagrangian for scalar fields, the local terms are automatically gauge invariant if the potential is a function $\phi^\dagger\phi$ (as it would be).

Not so for the kinetic terms, but we saw in the previous lecture that combinations

$$\phi^\dagger(x)U(x,y)\phi(y),$$

are gauge invariant.

We can make $\phi^\dagger(x)t_{\pm\mu}\phi(x)$ gauge invariant simply by inserting the parallel transporter along the link: $t_{\pm\mu}\phi(x) \to T_{\pm\mu}\phi(x) = U(x, x \pm ae^{(\mu)})\phi(x \pm ae^{(\mu)})$.

Lattice Gauge Fields

This means that the basic variables for lattice gauge fields are

$$U_\mu(x) = U(x, x + ae^{(\mu)}), \qquad U(x, x - ae^{(\mu)}) = U^\dagger(x - ae^{(\mu)}, x) = U_\mu^\dagger(x - ae^{(\mu)})$$

They take values in a Lie group. $\qquad\qquad\qquad A_\mu$ takes values in the Lie algebra.

So integrating over all $U_\mu(x)$ sums over all possible lattice gauge fields.

What is the measure? We want

$$\int dU\, f(U) = \int dU\, f(gU) = \int dU\, f(Ug^{-1}) \Rightarrow \int dU\, U = 0$$

$$\int dU\, 1 = 1 \Rightarrow \int dU\, U_{ij} U_{lk}^* = \frac{1}{N}\delta_{il}\delta_{kj} \quad \text{for SU}(N)$$

Mathematicians call this Haar measure.

Now we need an action for lattice gauge fields. The simplest one is obtained by analogy with the simplest action for scalar fields. Now the translations are

$$T_\mu U_\nu(x) = U_\mu(x) U_\nu(x + ae^{(\mu)}) U_\mu^\dagger(x + ae^{(\nu)})$$

$$T_{-\mu} U_\nu(x) = U_\mu^\dagger(x - ae^{(\mu)}) U_\nu(x - ae^{(\mu)}) U_\mu(x - ae^{(\mu)} + ae^{(\nu)})$$

So,

$$-\sum_{x,\mu} \mathrm{tr}[U_\nu^\dagger(x)(T_\mu + T_{-\mu} - 2)U_\nu(x)] = 2\sum_{x,\mu} P_{\mu\nu}$$

$$P_{\mu\nu} = \mathrm{Re}\,\mathrm{tr}[1 - U_\mu(x) U_\nu(x + ae^{(\mu)}) U_\mu^\dagger(x + ae^{(\nu)}) U_\nu^\dagger(x)].$$

and

$$S = \frac{\beta}{2N} \sum_{x,\mu,\nu} P_{\mu\nu}(x) \qquad \text{the Wilson (plaquette) action}$$

Exercise: show that the plaquette action reduces to the Yang-Mills action when $a \to 0$.